Vol 14 No 8, August 2005
1009-1963/2005/14(08)/1554-05

Chinese Physics

© 2005 Chin. Phys. Soc.
and IOP Publishing Ltd

Relativistic energy, fine structure and hyperfine structure of the low-lying excited states for Be-like system*

Zhang Meng(张 孟)† and Gou Bing-Cong(苟秉聪)

Department of Physics, Beijing Institute of Technology, Beijing 100081, *China*

(Received 6 January 2005; revised manuscript received 7 March 2005)

Variational calculations are carried out with a multiconfiguration-interaction wavefunction on the $1s^2 2p2p\ ^1D^e$ and $1s^2 2p3p\ ^3P^e$ states to obtain the energies including the mass polarization and relativistic corrections for the beryllium isoelectronic sequence (Z=4–10). The oscillator strengths, transition rates and wavelengths are also calculated. Our results are compared with other theoretical and experimental data in the literatures. The fine structure and hyperfine structure of $1s^2 2p3p\ ^3P^e$ state are also explored.

Keywords: Beryllium-like ion, variational calculation, fine structure, hyperfine structure
PACC: 3115, 3210, 3130

1. Introduction

In the past few decades, extensive theoretical researches[1−9] and experiments[10−13] have been done on the excited states of Be-like system. The relativistic energy and some of the fine structure and the hyperfine structure of Be-like system have been accurately determined in the past two decades by a variety of theoretical methods, such as the many-body perturbation theory methods,[14] the multiconfiguration Hartree–Fock method,[15−17] the variational calculations using multiconfiguration interaction wavefunctions,[18−20] and the multiconfiguration Dirac–Fock method.[21] However, to our knowledge, no calculations of the fine structure and the hyperfine structure for the $1s^2 2p3p\ ^3P^e$ have been reported. In our previous works, we have reported the hyperfine structure of the $1s^2 2p2p\ ^3P^e$ state,[20] in this work, we will extend to calculate the second root $^3P^e(2)$ and explore calculation of the fine and hyperfine structure for $1s^2 2p3p\ ^3P^e(2)$ state.

The purpose of this study is twofold: first, we calculated the energy levels of $1s^2 2p2p\ ^1D^e$ and $1s^2 2p3p\ ^3P^e$ states of the Be isoelectronic sequence (Z=4–10) with Rayleigh–Ritz variational and multiconfiguration-interaction method, and second, we investigate the fine structure, the hyperfine parameters, and the coupling constants of the excited state $1s^2 2p3p\ ^3P^e$ for the Be-like ions (Z=4–10). Our results will be useful for studying the observed spectra in future experiment.

2. Theories

The non-relativistic Hamiltonian for the Be-like ions, the four-electron system, is given in atomic units by

$$\hat{H}_0 = \sum_{i=1}^{4}\left[-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right] + \sum_{\substack{i,j=1\\ i<j}}^{4}\frac{1}{r_{ij}}. \tag{1}$$

The basic wavefunction $\psi_{\rm b}$ can be written as

$$\Psi_{\rm b}(1,2,3,4) = A\sum_i C_i \phi_{n(i),l(i)}(R) Y_{l(i)}^{LM}(\Omega)\chi_{SS_Z}, \tag{2}$$

where A is the antisymmetrization operator and the radial basis function are Slater orbitals:

$$\phi_{n(i),l(i)}(R) = \prod_{j=1}^{4} r_j^{n_j}\exp(-\alpha_j r_j). \tag{3}$$

The basic wavefunction $\psi_{\rm b}$ and the corresponding upper bound $E_{\rm b}$ are calculated by using the Rayleigh–

*Project supported by the National Natural Science Foundation of China (Grant No 10374008 and by the Doctoral Degree Program Foundation of Ministry of Education China (Grant No 20020007036), and by the BIT-UBF-200307A05.
†E-mail: manny@bit.edu.cn and goubing@sina.com

Ritz variation method.[18] To saturate the functional space, restricted variational method[22] is used to further improve the calculated value of energy $E_{\rm b}$. The total nonrelativistic energy is obtained by adding improvement from restricted variation $\Delta E_{\rm RV}$. In addition to $\Delta E_{\rm RV}$, the total energy is further improved by including the mass polarization effect and relativistic corrections, which are calculated by using first-order perturbation theory. The relativistic perturbation operators considered in this work are the corrections to the kinetic energy (P^4), the Darwin term, and the electron-electron contact term and orbit-orbit interaction. The operators of the relativistic and mass polarization perturbation are the same as those in Ref.[6]. The explicit expressions will not be repeated. Then the total energy becomes $E_{\rm total} = E_{\rm b} + \Delta E_{\rm RV} + \Delta E_{\rm rel}$.

For the fine structure, the perturbation operators are

$$H_{\rm SO} = \frac{Z}{2c^2}\sum_{i=1}^{4}\frac{l_i \cdot s_i}{r_i^3} \quad \text{(spin orbit)}, \tag{4}$$

$$H_{\rm SOO} = -\frac{1}{2c^2}\sum_{\substack{i,j=1\\ i\neq j}}^{4}\left[\frac{1}{r_{ij}^3}(r_i - r_j)\times P_i\right]\cdot(s_i + 2s_j)$$
$$\text{(spin other orbit)}, \tag{5}$$

$$H_{\rm SS} = \frac{1}{c^2}\sum_{\substack{i,j=1\\ i\prec j}}^{4}\frac{1}{r_{ij}^3}\left[s_i \cdot s_j - \frac{3(s_i \cdot r_{ij})(s_j \cdot r_{ij})}{r_{ij}^2}\right]$$
$$\text{(spin} - \text{spin)}. \tag{6}$$

These perturbations are calculated by using first-order perturbation theory.

The hyperfine interaction describes the interaction between the electrons and the magnetic and electric multiple moments of the nucleus. For an N-electron system, the hyperfine-interaction Hamiltonian is

$$H_{\rm hfs} = H_{\rm c} + H_{\rm SD} + H_{\rm l} + H_{\rm q}. \tag{7}$$

The hyperfine interaction couples the electronic angular momenta $\boldsymbol{J}$ and the nuclear angular momenta $\boldsymbol{I}$ to a total angular momentum $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{J}$. The explicit expressions of the hyperfine parameters (Fermi contact $a_{\rm C}$, the spin-dipolar $a_{\rm SD}$, the orbital $a_{\rm l}$, the electric quadrupole $b_{\rm q}$ and the coupling hyperfine constants $A_{\rm J}$, and $B_{\rm J}$) are the same as those in Ref.[16] and Ref.[23].

3. Results and discussion

The Be-like ions are the complex four-electron atomic system in which both intrashell and intershell state interactions are important. For this reason, in order to make sure that all important combinations are included in the basis function, we have made efforts to avoid missing an important contribution for a particular coupling. In this work, the number of angular-spin components in the basic wavefunctions ranges from 42 to 51 and the number of linear parameters in the basic wavefunctions ranges from 1022 to 1108. The energies are further improved by the restricted variational method with $\Delta E_{\rm RV}$ ranging from –74.7 to –96.8μa.u. To further improve the energy, the relativistic corrections and mass polarization are also included by using first-order perturbation theory.

In Table 1, we give the relativistic energies of the excited states $1s^2 2p2p\ {}^1D^e$ of the Be isoelectronic sequence (Z=4–10). For all cases, the nonrelativistic energies in this work are lower than those of Jonsson with MCHF calculations,[3] the improvement ranging from 0.0013 a.u. to 0.0078 a.u. Moreover, our theoretical results of relativistic energy levels including the mass polarization and relativistic perturbation are in good agreement with experiment[12,24–26] and other theoretical results[2,4,5,7] as shown in Table 1. The largest discrepancies between the obtained results of this work and those of the FCPC results[7] and the experimental results [12,24–26] are nearly 1% and 0.9% respectively. For the beryllium isoelectronic sequence, Table 1 shows that the differences between the CIV3[2] and the MBPT[4] calculations and the experimental results[12,24–26] decrease with increasing Z, the differences between the FCPC[7] calculations and the experimental results[12,24–26] increase with increasing Z, and the differences between this work and the BP[5] calculations and the experimental results [12,24–26] are almost the same with increasing Z. In general, for the multiconfiguration-interaction method, in a low-Z system, it is more difficult to calculate an accurate energy since the correlation and configuration-interaction effects between the electrons are stronger than those in a high-Z system. On the other hand, for relativistic effects, with increasing Z, relativistic effects become increasingly important. In the high-Z system, the higher-order relativistic effect, nuclear size effect and QED effect need to be considered for obtaining more accurate energies. Table 2 gives the relativistic energies and the fine structure energies relative to the ground state of the excited states $1s^2 2p3p\ {}^3P^e$ of the Be isoelectronic sequence (Z=4–10). The

unpublished NIST data (http://physics.nist.gov/cgi-bin/AtData) of the fine structure energies relative to the ground state of the excited states $1s^22p3p\ ^3P^e$ (in cm^{-1}) are also given for comparison in Table 2. It can be seen that the differences between our calculated data and NIST data are very small. The maximum difference between our calculated and NIST data is approximately 0.5% of Be_I, and as the nuclear charge number increases, this difference will be less than the pronounced value and will reach approximately 0.08% of Ne_{VII}.

Table 1. Relativistic energies (in a.u.) of the low-lying excited states $1s^22p2p\ ^1D^e$ of the Be isoelectronic sequence. T is the term energy levels (in cm^{-1}).

Z	E_{nonrel}		E_{total}	T/cm^{-1}						
	this work	MCHF[3]	this work	this work	BP[5]	MBPT[4]	CIV3[2]	FCPC[7]	Exp.	NIST*
				$1s^22p2p\ ^1D^e$						
4	−14.406925	−14.406795	−14.409143	57202		51665			56432[a)]	56882
5	−23.881069	−23.880826	−23.886945	102396	103671	98608	103557	102248	102362[a)]	102363
6	−35.869376	−35.868799	−35.882415	146339	146794	143146	146504	145633	145876[b)]	145876
7	−50.362568	−50.361781	−50.388132	189364	190235	186764	189610	188324	188882[c)]	188882
8	−67.357840	−67.357560	−67.402775	232474	233350	230003	232177	230632	231721[d)]	231721
9	−86.855512	−86.855089	−86.929845	275428	276488	273165	274478	272689	274597[a)]	274602
10	−108.853965	−108.853786	−108.970496	318639	319868	316463	316560	314578	–	319720

[a)] Ref.[12], [b)] Ref.[24], [c)] Ref.[25], [d)] Ref.[26].

*(http://physics.nist.gov/cgi-bin/AtData/)

Table 2. Relativistic energies (in a.u.) and the fine structure energies (in cm^{-1}) of the excited states $1s^22p3p\ ^3P^e$ of the Be isoelectronic sequence.

Z	E_{nonrel}	E_{total}	T/cm^{-1}						
	this work			this work			NIST*		
	$1s^22p3p\ ^3P^e$			J=0	J=1	J=2	J=0	J=1	J=2
4	−14246136	−14248258	92486	92484	92485	92487	92014	92015	92018
5	−23455505	−23461323	196188	196176	196182	196194	195610	195611	195614
6	−35031923	−35044850	330156	330117	330137	330174	329685	329706	329743
7	−48971398	−48996479	494785	494688	494738	494831	494253	494309	494402
8	−65273441	−65317916	690032	689829	689984	690131	689403	689517	689708
9	−83937221	−84010682	916091	915713	915908	916276	915180	915403	915760
10	−104962656	−105077331	1173066	1172419	1172752	1173383	117200	1172140	1172470

*(http://physics.nist.gov/cgi-bin/AtData/)

Table 3 gives computed oscillator strengths from the dipole length (f_l), dipole velocity (f_v), and dipole acceleration (f_a) formulae[22] and the transition wavelengths for $1s^22s2p\ ^1P^o$–$1s^22p^21D^e$ and $1s^22s2p\ ^3P^o$–$1s^22p3p^3P^e$. As Table 3 shows, in this work the f_l, f_v, and f_a are in good agreement with each other. For example, the f_l, f_v, and f_a of transition $1s^22s2p\ ^1P^o$–$1s^22p2p\ ^1D^e$ in N_{IV} are 0.1703, 0.1704 and 0.1751 respectively. The good agreement between the length, velocity and acceleration results could be used as the indication of the accuracy of the wavefunctions. The results of our calculations are in perfect agreement with the results of the other theoretical calculations[2,3,7,27] which only gave the values of the f_l and f_v. The differences of the f_l and f_v from this work and CIV3 calculations,[2] MCHF calculations[3] and FCPC calculations[7] are approximately 1.8%, 0.95% and 0.55% or less respectively. In Table 3 we also compared the calculated $1s^22s2p\ ^1P^o$–$1s^22p^21D^e$ and $1s^22s2p\ ^3P^o$–$1s^22p3p^3P^e$ transition wavelengths with those of the NIST data, For most of our results, the transition wavelengths of this calculation are in good agreement with those of the NIST data. However, for Be_I, our result is slightly higher than that of the NIST data (see Table 3).

Table 3. Comparison of the oscillator strengths (f_l, f_v) and transition wavelengths (nm) for $1s^22s2p\ ^1P^o$–$1s^22p^2\ ^1D^e$ and $1s^22s2p\ ^3P^o$–$1s^22p3p\ ^3P^e$ of the Be-like isoelectronic sequence.

Z	$1s^22s2p\ ^1P^o \rightarrow 1s^22p2\ ^1D^e$							
	$f_l/\ f_v/f_a$					λ/nm		
	This work	MCHF[3]	CIV3[2]	FCPC[7]	Opacity[25]	This work	MCHF[3]	NIST*
4	0.0001/ 0.0001/ 0.0002	0.0002/ 0.0004				712.53	705.15	698.27
5	0.1615/ 0.1612/ 0.2141	0.1597/ 0.1568	0.1850/ 0.2007	0.1616/ 0.1606	0.1557	347.41	347.51	345.12
6	0.1828/ 0.1793/ 0.2088	0.1799/ 0.1776	0.1920/ 0.1947	0.1811/ 0.1803	0.1800	228.93	231.16	229.87
7	0.1703/ 0.1704/ 0.1751	0.1698/ 0.1681	0.1750/ 0.1723	0.1706/ 0.1701	0.1710	171.44	173.08	171.86
8	0.1563/ 0.1542/ 0.2130	0.1552/ 0.1539	0.1577/ 0.1548	0.1556/ 0.1553	0.1567	136.41	138.39	137.12
9	0.1418/ 0.1405/ 0.2161	0.1410/ 0.1401	0.1420/ 0.1370			114.35	115.46	113.95
10	0.1292/ 0.1282/ 0.2125	0.1285/ 0.1277	0.1295/ 0.1224	0.1288/ 0.1286	0.1297	96.91	98.94	–
	$1s^22s2p\ ^3P^o \rightarrow 1s^22p3p\ ^3P^e$							
4	0.0001/ 0.0001/ 0.0001					143.44		
5	0.0102/ 0.0095/ 0.0085					63.61		
6	0.0262/ 0.0261/ 0.0265					36.44		36.08
7	0.0416/ 0.0412/ 0.0418					23.74		23.41
8	0.0538/ 0.0535/ 0.0534					16.75		16.46
9	0.0639/ 0.0637/ 0.0642					12.48		
10	0.0723/ 0.0721/ 0.0736					9.68		

*(http://physics.nist.gov/cgi-bin/AtData/)

Table 4 gives the shifts of the various J levels (ΔE_J) from the center-of-gravity energy and the fine-structure splittings ($\nu_{J-J'}$) of $1s^22p3p\ ^3P^e$ state. In this work, the fine-structure splittings of the triplet states $1s^22p3p\ ^3P^e$ are calculated by using first-order perturbation theory. If including the effects of the spin–orbit, spin–other-orbit and spin–spin interactions, we obtain the energy of the fine structure resolved J levels as given in Table 2. In Table 5 we give Fermi contact a_C, the spin-dipolar a_{SD}, the orbital a_l, and the electric quadrupole b_q hyperfine structure parameters and the hyperfine coupling constants A_J and B_J for the $1s^22p3p\ ^3P^e$ states of the different beryllium-like species. In this calculation, the nuclear spin $\boldsymbol{I}$, the nuclear magnetic dipole moment μ_I, and the electric quadrupole moment Q are taken from Ref.[28]. To our knowledge, no calculations of the fine structure and the hyperfine structure have been reported for the triplet excited states $1s^22p3p\ ^3P$ of the beryllium-like isoelectronic sequence in the literatures. So we cannot make any comparison with other theoretical and experimental results and we hope that our results should be useful for the experiments in the future.

Table 4. Center-of-gravity total energies E_{CG} (in a.u.), fine structure corrections ΔE_J (in a.u.) and fine structure splittings $\nu_{J-J'}$ (in cm^{-1}) of $1s2s2p3p\ ^3P^e$ low-lying excited states of the Be-like isoelectronic sequence.

Species	E_{CG}	$\Delta E_{J=1}$	$\Delta E_{J=2}$	$\Delta E_{J=3}$	ν_{1-0}	ν_{2-1}
^{9}Be	–14.2482576	–0.0000099	–0.0000048	0.0000048	1.14	2.10
^{11}B	–23.4613229	–0.0000540	–0.0000256	0.0000262	6.24	11.36
^{11}C	–35.0448498	–0.0001774	–0.0000843	0.0000860	20.42	37.38
^{14}N	–48.9964794	–0.0004405	–0.0002114	0.0002149	50.27	93.56
^{17}O	–65.3179158	–0.0009220	–0.0004447	0.0004512	104.76	196.62
^{20}F	–84.0106822	–0.0017186	–0.0008321	0.0008430	194.56	367.62
^{22}Ne	–105.0773314	–0.0029437	–0.0014281	0.0014456	332.64	630.67

Table 5. The hyperfine parameters (in a.u.) and coupling constants (in MHz) of 1s2s2p3p $^3P^e$ state for Be-like isoelectronic sequence.

Species	a_c	a_{SD}	a_l	b_q	A_J		B_J	
					J=2	J=1	J=2	J=1
^{9}Be	–1.17133	0.05371	0.25361	0.09936	0.00313	0.01521	–0.00124	0.00062
^{11}B	–2.73118	0.17546	0.84606	0.32711	0.00943	–0.08070	–0.00312	0.00156
^{11}C	–5.26526	0.40780	1.97636	0.76927	–0.01924	0.05587	–0.00619	0.00310
^{14}N	–7.83572	0.78270	3.80617	1.49791	0.03804	–0.05253	–0.00679	0.00340
^{17}O	–11.65832	1.32486	6.49511	2.54612	–0.14205	0.14555	0.01542	–0.00771
^{20}F	–14.98691	2.08954	10.20512	4.00721	0.36430	–0.26248	–0.03955	0.01977
^{22}Ne	–17.48835	3.08722	15.09842	5.95220	–2.22209	1.11392	–	–

References

[1] Fleming J, Vaeck N, Hibbert A, Bell K L and Godefroid M R 1996 *Phys. Scr.* **53** 466

[2] Fernly J A, Hibbert A, Kingston A E and Seaton M J 1999 *J. Phys.* B **32** 5507

[3] Jonsson P, Fischer C F and Godefroid M R 1999 *J. Phys.* B **32** 1233

[4] Safronova M S, Johnson W R and Safronova U I 1996 *Phys. Rev.* A **53** 4036

[5] Kingston A E and Hibbert A 2002 *J. Phys.* B **33** 693

[6] Chung K T, Zhu X W and Wang Z W 1993 *Phys. Rev.* A **47** 1740

[7] Zhu X W and Chung K T 1995 *Phys. Scr.* **52** 654

[8] Wang F, Gou B C and Han L H 2001 *Acta Phys. Sin.* **50** 1685 (in Chinese)

[9] Gou B C, Yu K Z, Wang F and Wu X L 2003 *Chin. Phys.* **12** 951

[10] Kelly R L 1987 *J. Phys. Chem. Ref. Data* **16** suppl. No 1

[11] Edlen B 1983 *Phys. Scr.* **28** 51

[12] Moore C E 1971 *Atomic Energy Levels NBS Circular* **1** No 467

[13] Trabert E 1991 *Phys. Sci.* **41** 675

[14] Ray S N, Taesul L and Das T P 1973 *Phys. Rev.* A **7** 1469

[15] Sundholm D and Olsen 1991 *J. Chem. Phys. Lett.* **177** 1469

[16] Carlsson J, Jonsson P and Fischer C F 1992 *Phys. Rev.* A **46** 2420

[17] Jonsson P and Fischer C F1993 *Phys. Rev.* A **48** 4113

[18] Yang H Y and Chung K T1995 *Phys. Rev.* A **51** 3621

[19] Wang F and Gou B C 2003 *J. Phys.* B **36** 331

[20] Wang F, Gou B C, Wu X L and Han L H 2003 *Int. J. Mod. Phys.* C **14** 549

[21] Marques J P, Parente F and Indelicato P 1993 *Phys. Rev.* A **47** 929

[22] Chung K T and Gou B C 1995 *Phys. Rev.* A **52** 3669

[23] Hibbert A 1975 *Rep. Prog. Phys.* **38** 1217

[24] Moore C E 1970 *Selected Tables of Atomic Spectra* (Washington, DC: Govt Printing Office) Circ. No.3, Sec. 3

[25] Moore C E 1971 *Selected Tables of Atomic Spectra* (Washington, DC: Govt Printing Office) Circ. No.3, Sec. 4

[26] Moore C E 1980 *Selected Tables of Atomic Spectra* (Washington, DC: Govt Printing Office) Circ. No.3, Sec. 9

[27] Seaton M J 1996 *The Opacity Project* (Bristol: IOP Publishing) Vol.1

[28] Raghavan P 1989 *At. Data Nucl. Data Tables* **42** 181